Nano-Indentation of Copper – Nickel thin films

-A Molecular Dynamics Simulation Study

A Thesis submitted in partial fulfillment of the requirements for the Degree of
Bachelor of Technology (B. Tech)
In
METALLURGICAL & MATERIALS ENGINEERING

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CERTIFICATE

This is to certify that the project entitled "**Nano-indentation study of Copper-Nickel thin films- A Molecular Dynamics Simulation Study**" submitted by **Mr. SIDDHARTH MISHRA (109MM0478) and Mr. BIPIN KUMAR SETHY (109MM0459)** in partial fulfillments for the requirements for the award of **Bachelor of Technology** Degree in **Metallurgical & Materials Engineering** at **National Institute of Technology, Rourkela** (Deemed University) is an authentic work carried out by them under my supervision and guidance.

To the best of my knowledge, the matter embodied in the report has not been submitted to any other University / Institute for the award of any Degree or Diploma.

Date: 08.05.2013

Prof. N. Yedla
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ACKNOWLEDGEMENT

We would like to thank **NIT Rourkela** for giving us the opportunity to use its resources and work in such a challenging environment. First and foremost, we take this opportunity to express our deep regards and sincere gratitude to our guide **Prof. N. Yedla** for his able guidance and constant encouragement during our project work. This project would not have been possible without his help and the valuable time that he has given us amidst his busy schedule.

We would also like to express our utmost gratitude to **Prof. B.C Ray, HOD, Metallurgical & Materials engineering** for allowing us to use the departmental facilities and for his valuable suggestions and encouragements at various stages of the work.

We would also like to extend our hearty gratitude to our friends and senior students of this department who have always encouraged and supported in doing our work. Last but not the least; we would like to thank all the staff members of Department of Metallurgical &Materials Engineering who have been very cooperative with us.

Place: NIT-Rourkela

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ABSTRACT

Nanostructured materials have attracted many attentions and have been the subject of intensive research in recent years because they possess novel and/or enhanced mechanical properties compared with coarse grained materials. These enhanced mechanical properties of nanomaterial are an important subject of Nano-mechanics research. When brought into a bulk scale, nanoparticles can strongly affect the mechanical properties of the material, like stiffness or elasticity. The mechanical behaviour of very small volumes differs from what is typically observed on the macro level. In particular, thin metal films with nanometer-sized coatings possess interesting mechanical properties.

Here, we have used molecular dynamics simulations to elucidate effect of Ni-thickness, effect of loading rate, effect of temperature on load-displacement behaviour during nano-indentation of thin copper films with nickel coatings. After simulation is being performed several deformation mechanisms, such as pile-up of dislocation at the interface, edge dislocation slip lines are observed. Most interestingly, the underlying copper films or substrates are significantly strengthened by thin nickel coatings. The strengthening effect is more pronounced at a low temperature.

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Chapter-1

Introduction

1.1 Introduction to nano thin films:

Now-a-days, the overwhelming advancement of science and technology has paved the way for scientists to find out new materials for high technology applications. During the past decade specific property material requirements for advanced applications have escalated where conventional material systems are not suitable. The materials used for high technology applications are designed to have maximum performance at optimum conditions. Some of the modern engineering materials which have attracted considerable attention of material scientists are nano structured materials, super alloys, metallic glasses, shape memory alloys (SMA), carbon nanotubes various MMCs (Metal Matrix Composites) etc. Here the focus of this project work is on the nano thin films.

In a lay man view, nanomaterial is a field that takes a materials science-based approach on the concept of nanotechnology. Since last few decades it has earned huge importance. It studies materials with nanoscale morphological features, and specifically those that have special properties stemming from their nanoscale dimensions and extremely small grain sizes. Nanoscale regime is usually defined as smaller than a one tenth of a micrometer in at least one dimension [1] though this term is sometimes used for even smaller materials. A thin film is a layer of material ranging from fractions of a nanometer (monolayer) to several micrometers in thickness. These are very thin layers of materials used to manipulate various surface properties.

The beginning of “Thin Film Science” can possibly be traced to the observations of Grove [2] who noted that metal films were formed by sputtering of cathodes with high energy positive ions bombardment to the target material. Since then it has attracted many attentions and come a long way and today it is no longer a subject of some casual academic interest but has become a full-fledged discipline. The phenomenal rise in thin film researches is no doubt due to their

extensive applications in the diverse fields and advanced industrial applications. These investigations have led a numerous inventions in the forms of active devices and passive components, piezo-electric devices, micro-miniaturized application of power supply, rectifying and amplifying instruments, sensor components, storage equipments of solar energy and its abilty to convert to other form, magnetic memories, super conduction films, interference filters, reflecting and antireflection coatings and many others.

1.2 Properties of Nanostructured Materials:

Since last few years Nanostructured materials have gained so much importance and have been the subject of intensive research because they exhibit unique mechanical properties [3]. Some known physical properties of nano-materials are related to different origins; for example,

(i) Large fraction of surface atoms

(ii) Large surface energy due to high surface to volume ratio.

(iii) Spatial confinement

(iv) Reduced imperfections.

- Mechanical properties of nano materials may reach theoretical values, which may be several orders of magnitude higher than that of single crystals in the bulk form. This can be attributed to the reduced probability of defects.
- Optical properties of nanomaterials can be significantly different. For example, the optical absorption peak of a semiconductor nano-particle shifts to a short wavelength due to increased band gap.
- Electrical conductivity decreases due to reduced dimension giving rise to surface scattering however it can be increased significantly due to the better ordering in microstructure.

- Ferromagnetism of bulk materials dissolves and instead transforms to superparamagnetism in nanoscale regime due to high surface energy.

1.3 Deformation Mechanism in Nano thin films:

In coarse-grained materials, the main carrier of plastic deformation is nucleation of dislocations from Frank– Read sources and their subsequent motion through individual grains. Grain boundaries act as a barrier and hinder dislocation activity and create dislocation pile-ups, thus making metal harder to deform. Reduction in the grain size creates more grain boundaries thus creating more obstacles to dislocation motion and usually results in strengthening of polycrystals. This increase in yield stress is found to be inversely proportional to the square root of the grain size (known as the Hall–Petch relation [4, 5]). However, at very small grain sizes the Hall–Petch relation breaks down and even becomes a reverse one. Initiated by experimental observations [6], molecular dynamics simulations of Schiøtz et al. [7] found a reverse Hall–Petch phenomenon (softening with decreasing grain size) in mechanical behaviour of nanocrystalline copper with grain sizes from 3.3 to 6.6 nm, thereby suggesting the existence of the strongest grain size [8,9,10]. This modification of material behaviour at a certain critical grain size is observed because new deformation mechanisms begin to operate at those regimes. Specifically, since in case of nanocrystalline materials grain boundaries form a substantial fraction of the material because of very small grains. Dislocations are primarily observed in larger grains and often are immobile. Therefore, the plastic deformation in nanocrystals is no longer carried by dislocations; it is believed to be a result of grain boundary accommodation mechanisms [7-11, 12, 13].

1.4 Production Techniques:

These films are solid and typically either metallic or compounds. Thin films can be made by a variety of techniques. Each of these techniques has their own advantages and disadvantages. Few of them are discussed below briefly.

1. Electro deposition:

   Also referred to as electroplating in which the used electric current reduces the dissolved metal cations so that they form coherent coatings of metal on an electrode.

   Advantages:

   - Low temperature treatment
   - High hardness
   - Low friction
   - Most versatile to a wide range of substrates
   - Thick layers possible

   Disadvantages:

   - Thickness uniformity is not maintained on complex parts.
   - Hydrogen embrittlement
   - Not stands good when the substrate is insulating
   - plating baths may arise environmental concerns

2. Conversion coating:

Thin compound layers can be produced by reacting a metal surface with an acidic solution. These acids ensure low friction surfaces with some resistance to adhesive wear.

Advantages:

- Cheap and simple to perform
- Low temperature treatment

Disadvantages:

- Entire range of materials can't be treated
- Thin treated layer
- Poor treatment durability
- Control of treatment quality is not feasible.

3. Chemical Vapour Deposition(CVD):

It is used to produce high quality and high strength solid materials. In this process, the substrate is exposed to one or more volatile precursors, which subsequently react and/or decompose on the substrate surface resulting the desired deposit. Mostly, volatile by-products are also produced that are removed by gas flow through the reaction chamber.

Advantages:

- High coating hardness
- Good adhesion (if the coating is not too thick) & good throwing power.

Disadvantages:

- High temperature process (distortion)
- Sharp edge coating is difficult (thermal expansion mismatch stresses)
- Entire range of materials can't be coated
- process gases may cause environmental problems

4. Physical Vapour Deposition(PVD):

This is class of coating method that involves purely physical processes such as high temperature vacuum evaporation along with subsequent condensation, or plasma sputter bombardment rather than involving a chemical reaction at the surface to be coated as in chemical vapor deposition.

Advantages:

- Excellent process control
- Low deposition temperature
- Dense, adherent coatings
- Elemental, alloy and compound coatings possible

Disadvantages:

- high capital cost
- Limited component size treatable
- Relatively low coating rates

5. Sputtering:

Sputtering is itself a PVD process in which atoms are ejected from a solid target material when the target is bombarded by high energy materials when the kinetic energy of the incoming particle is much higher than thermal energies.

6. Ion implantation:

It is a vacuum process in which ions are injected into a surface when a beam of ions is directed at that surface. These directed ions lose energy in collisions with the target atoms and come to rest in the surface layer of the material with an approximately Gaussian distribution.

Advantages:

- Low temperature process
- Very versatile - every stable element in the periodic table can be implanted into any vacuum compatible target
- Highly controlled
- No distortion - can be applied to finished components

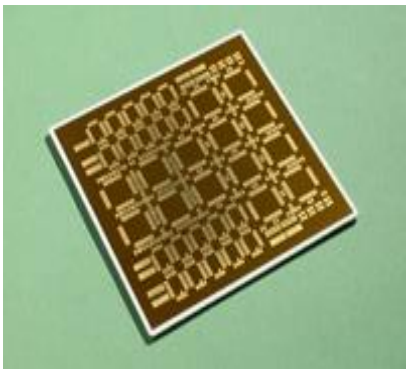
Disadvantages:

- Line of sight process
- Expensive vacuum equipment needed
- Very thin treated layer

1.5 Thin films applications:

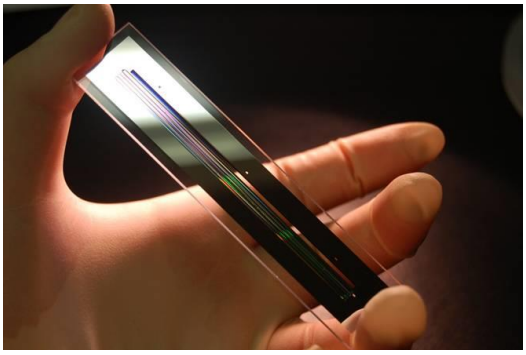
Thin films have significant importance in a large variety of industrial applications. This technology is available for the purpose of tailoring coating materials for specific property applications. Some of the widely used applications are mentioned below briefly.

- Microelectronics - electrical conductors, electrical barriers, diffusion barriers etc.
- Magnetic sensors - sense I, B or changes in them
- Gas sensors, SAW devices
- Tailored materials – layer of very thin films to develop materials with new properties
- Optics - anti-reflection coatings
- Fabrication of materials having high Corrosion resistant and wear resistant.



Multi-chip Thin Film over a Ceramic Substrate

Thin-Film Photovoltaic



Optical coating

Fig. 1.1. Some potential applications of thin films

A lot of work has also been reported on magnetic application of thin films including synthesis of piezoelectric and ferroelectric thin films. Many researches have also been performed to study the effect of shrinking the material in one or more directions and as a result how the properties can be tailored for advance applications. And also they have developed techniques for extremely well controlled growth of thin films and usage of computer modeling for predicting physical and chemical properties of thin films materials.

So in this project work, our main objective is to study the deformation behavior of Cu-Ni thin films during nano-indentation through molecular dynamics simulation studies. This sample has been chosen because they have shown enhanced hardness behaviour [14] and have even displayed the so-called supermodulus effect [15].

Chapter-2

Literature Review

2. Literature Review:

Denis Saraev and Ronald E. Miller [20] from Department of Mechanical and Aerospace Engineering, Carleton University, Canada have studied on atomic scale simulations of nanoindentation-induced plasticity in copper crystals with nano-meter sized Ni-coatings. They have used molecular dynamics simulations to elucidate details of plastic deformation and the underlying deformation mechanisms during nanoindentation of thin copper films with epitaxial nickel coatings. They have studied the effect of Ni-thickness and indenter size on change in hardness of the bulk Cu crystal due to Ni coatings. They have plotted load v/s displacement curves for indentation on different thicknesses of Ni coatings to deduce the results.

Wen-Yang Chang, Te-Hua Fang, Shiang-Jiun Lin and Jian-Jin Huang [21] have investigated nanoindentation response of Ni surface using molecular dynamics simulations. The mechanisms of dislocation nucleation on a nickel (Ni) (001) surface under nanoindentation is investigated using MD simulation. The multi-step load/unload cycles on the Ni atoms were investigated in order to attain better explanation of the influence of the models, the tilt angles and geometry on the material's behaviour under nanoindentation. This study shows how molecular dynamics (MD) simulation for nanotechnology analyses of atomistic models has been used to further clarify the dislocation and defect structures. The MD method can be effective in simulating the atomistic characteristics of deformation and microscopic fracture processes, and offering insights into microscopic behaviours.

Cheng-Liang Liu, Te-Hua Fang, Jen-Fin Lin [22] have studied atomistic simulations of hard and soft films under nanoindentation. Three-dimensional molecular dynamics (MD) simulation is used to investigate the atomistic mechanism of nanoindentation process under

different temperature, indentation load and loading rates of indenter. The hard materials mainly selected are diamond and soft materials as gold. The results showed that when the loads and the loading rates were increased, both the modulus of elasticity and the hardness of the films were increased. When the nanoindentation was done under high temperatures, the thermal softness behaviour took place causing a reduction in Young's modulus. Due to the improvements in manufacturing technology, the thickness of films used for semiconductors or micro devices has been reduced to the nano-meter level. However, there is a marked difference between the mechanical characteristics of bulk materials and Nano-films. In order to clearly understand these differences in mechanical characteristics, it is necessary to investigate the physical properties of thin films. Nanoindentation is the most continually used technique for measuring various properties of thin films.

E.T. Lilleodden, J.A. Zimmerman, S.M. Foiles, W.D. Nix [**23**] studied the Atomistic simulations of elastic deformation and dislocation nucleation during nanoindentation. In this work, a simulation study of the initial stages of indentation using the embedded atom method (EAM) is presented. The principles of the EAM are listed, and a comparison is made between atomistic simulations and continuum models for elastic deformation. Then, the analysis is done for the mechanism of nucleation of dislocation in single crystalline gold materials, and the effects of elastic anisotropy are considered. The EAM method is based upon the recognition that the cohesive energy of a metal is governed not only by the pairwise potential of nearest neighbour atoms, but also by the embedding energy related to the "electron sea" in which the atom is embedded. In this work typical load–displacement data generated during simulation shows elastic behaviour as well as discrete drops in the load associated with dislocation nucleation. These load drops are analogous to the displacement bursts during load-controlled experiments.

Arun K. Nair, Edward Parker, Peter Gaudreau, Diana Farkas, Ronald D. Kriz [24] did work on the effects of size in indentation response of thin films at nanoscale. They have studied the indentation response of Ni thin films of thicknesses in the nanoscale using molecular dynamics simulations with embedded atom method (EAM) interatomic potentials. They have performed a series of simulations in films in the [1 1 1] orientation with thicknesses varying from 4 to 12.8 nm. The investigation included both single crystal films along with the films containing low angle grain boundaries perpendicular to the surface of the film. The obtained simulation results for single crystal films show that as film thickness decreases larger forces are required for similar indentation depths but the contact stress necessary to emit the first dislocation under the indenter is nearly independent of film thickness. Most of the times the low angle grain boundaries act as sources of dislocation during indentation. The mechanism of emission of preferred dislocation from these boundaries operates at stresses that are lower as the film thickness increases and is not active for the thinnest films tested.

A. Hasnaoui, P.M. Derlet, H. Van Swygenhoven [25] have done work on interaction between dislocations and grain boundaries under an indenter using molecular dynamics simulation. They have used Large-scale molecular dynamics simulations of nanocrystalline Au to investigate the interaction between dislocations emitted under an indenter and the nearby grain boundary network. They have shown that for cases where the indenter size is smaller than the grain size, grain boundaries not only act as a sink for dislocations, but that depending on their local structure and stress distribution, they can also reflect or emit dislocations. The emission and absorption process is accompanied by local atomic activity involving atomic shuffling and free volume migration within the grain boundary region.

Shuai Shao [26] in his work have studied the deformation mechanism in nanoscale multi-layered metallic composites. The motive of his work is to have clear understanding the interaction between dislocations and various metallic interfaces in nanoscale metallic multilayers (NMM). At lower strain rates, this mean understanding the effect of interfaces to the strain hardening of the NMMs; at higher strain rates, this means the effect of the interfaces on the spallation strengths of the NMMs. NMMs show ultra-high strength level which is owing to the interactions between single dislocations (i.e. no pile-up) and interfaces. Nanoindentation simulations are implemented at a low strain rates on a series of Cu-Ni-Nb bases metallic nano layers. Through this simulations the mechanism of interaction of dislocations with single interfaces in a rather isolated environment are investigated. Strengthening mechanism of metallic multi layers is examined. The work have suggested that this strengthening effect is due to the presence of the interface between two dissimilar materials or the strengthening can be the result of following four mismatches between the adjacent layers: elastic modulus, lattice parameter, gamma surface (chemical) and slip-plane.

Chapter-3

Computational Methods

3.1 Introduction to Modeling and Simulations

3.1.1 Model:

It can be defined as a simplified exhibition of a system at some particular instant of time or space with an objective to promote understanding of the real system.

TYPES OF MODELS:

1. Atomistic Modeling
2. Monte carlo
3. Continuum

Atomistic simulation models materials at the level of atoms using modern computing power to explicitly include every atom in the model. Since interacting atoms are the foundation and base of materials science, atomistic modeling has helped a lot in the field of computational materials studies. It can be classified broadly into two categories

1. Molecular statics
2. Molecular Dynamics

In Molecular statics the relaxed configuration (positions and velocities) of atoms is found by conjugate gradient method or some similar energy minimization method. These simulations provide information of crystal lattice structure in different phases and under different conditions [16].

In case of Molecular Dynamics the actual motion of atoms is simulated by evolving the atomic configuration (atomic positions and velocities) with time by integrating Newton's Equation of Motion [16].

Force = mass x acceleration

3.1.2 Simulation:

It is the manipulation of a model in such a way that it operates on time or space to compress it, thus enabling one to perceive the interactions that would not otherwise be apparent because of their separation in time or space.

3.2 Molecular Dynamics Simulation

3.2.1 Introduction:

Molecular dynamics (MD) is a computer simulation technique where the time evolution of a set of interacting atoms and molecules of a system is followed by integrating their equations of motion (F=ma). The atoms and molecules present in the system are allowed to interact for a period of time. The trajectories obtained of the interacting particles are determined by numerically solving Newton's equations of motion where forces between the particles and potential energy are defined by molecular mechanics force fields. The Newton's equation of motion can be expressed mathematically as follows:

$$F = m_i a_i \quad \text{..... (i)}$$

$$a_i = d^2 r_i / dt^2 \quad \text{..... (ii)}$$

Where F= interatomic force between the interacting particles

m_i= mass of each particle (considering a homogeneous system, mass of each particle is same)

a_i = Acceleration of each particle

r_i = particle position

Given an initial set of positions and velocities, the subsequent time evolution through which the particle interaction and movement takes place can be completely determined. During simulation atoms and molecules will 'move' in the computer, bumping into each other during

interaction, vibrating about a mean position (if constrained), or wandering around (if the system is fluid), oscillating in waves in concert with their neighbors, perhaps evaporating away from the system if there is a free surface, and so on, in a way similar to what real atoms and molecules would do.

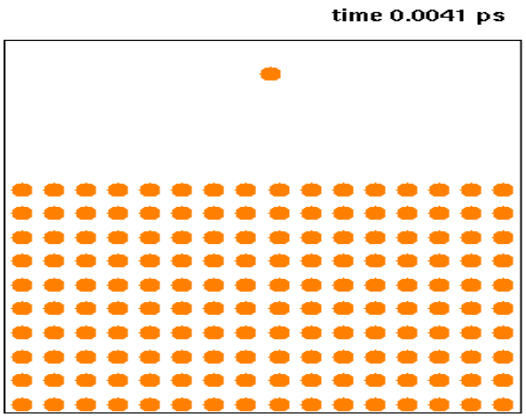


Fig. 3.1 Example of MD simulation in a simple system: Deposition of a single Cu atom over a Cu (001) surface. Each colored atom represents Cu atom [17]

The initialization of MD Simulation starts with initializing the position and velocities of atoms and after that the total energy is being calculated which includes bond energy, torsional energy, bond angle energy, non-bond energy. Then the forces on the atoms are calculated. Subsequently atoms are moved and newton's equation of motion is integrated to obtain the atomic trajectory.

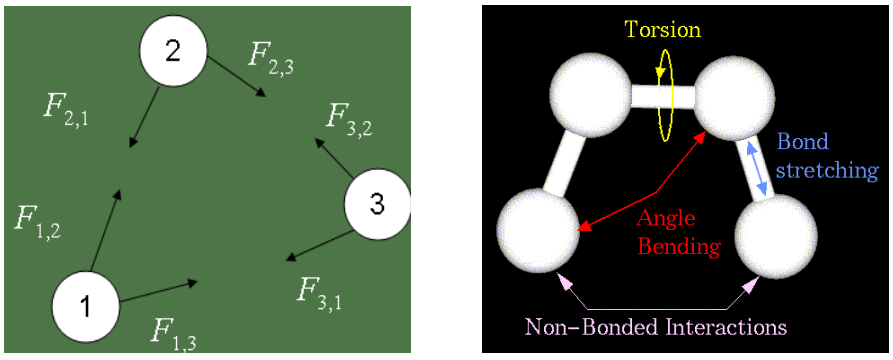


Fig 3.2 Figure showing various forces of interaction between atoms.

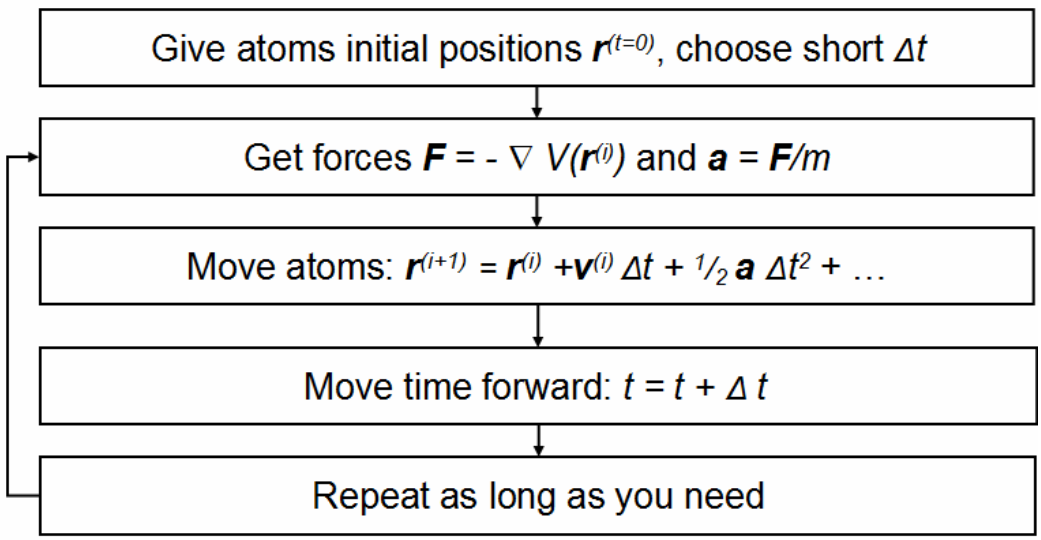


Fig 3.3. The process algorithm for Molecular Dynamics simulation [17]

Since any molecular system contains a large no of micro-particles, atoms or molecules, it is quite impractical and most of the times impossible to characterize the properties of such a vast system analytically. In this case MD simulation comes handy to solve this problem by using numerical methods. To achieve the simulation results that are error free, calculations are carried out by selecting a proper algorithm implemented in a suitable programming language in a machine (computer). Therefore, complexity can be introduced and more realistic systems can be examined, getting a better understanding of real experiments. Due to its important commercial applications in large scale, this kind of simulation technique is now gaining much more popularity.

3.2.2 Design Parameters in MD Simulation:

MD simulation facilitates the study on the dynamics of large macro-molecules along with the optimization of resulting structures. As discussed earlier the trajectory obtained by molecular dynamics as per the algorithm provided gives a set of conformations of molecule. As the simulation proceeds with atomic movements, thermodynamic parameters of the system like temperature, pressure, volume, total energy gets modified and finally we get the desired result as per the algorithm used. Based on these parameters, simulation can be done in various ways. They are as follows [18,27]:

Micro-canonical or NVE ensemble:

In this case, the system is restrained from changes in moles (N), volume (V) and energy (E). It corresponds to an adiabatic process with no heat exchange. A micro-canonical molecular dynamics trajectory may be considered as an exchange of potential energy and kinetic energy and where total energy is being conserved.

Canonical or NVT ensemble:

In this case, moles (N), volume (V) and temperature (T) are conserved in the system. Also sometimes called constant temperature molecular dynamics (CTMD). In NVT, the energy of endothermic and exothermic processes is exchanged with a thermostat. A variety of thermostat methods is available to add and remove energy from the boundaries of an MD system in a more or less actual way, approximately defining the canonical ensemble.

Isothermal–Isobaric or NPT ensemble:

In this case, moles (N), pressure (P) and temperature (T) are conserved. Along with a thermostat sometimes a barostat is needed to control the pressure to approximate real situation.

Design of a molecular dynamics simulation should be in accordance with available computational power. Various parameters like simulation size (n=number of particles), timestep and total time for simulation must be selected carefully so that the calculation can be finished within a reasonable time period.

Various factors affect the total simulation time and they should be taken into consideration. In the case of a classical MD simulation, the most important task of CPU is the evaluation of the potential (force field) as a function of the particles' internal coordinates. Calculations are more time-consuming, while encountering the non-bonded or non-covalent parts of a system.

Potential function or force field measures quantitatively how the particles will interact and represent a classical treatment of particle-particle interactions that results in structural and conformational changes but usually cannot reproduce chemical reactions. Various potentials that are widely used in simulation are given below and choice of potential depends on the user depending on the type of material system we are dealing with.

Empirical Potentials:

Those used in chemistry are frequently called force fields, but material physics gives it a different name. Most force fields in chemistry are empirical and consist of a summation of bonded forces associated with chemical bonds, forces due to bond angles, torsional forces and non-bonded forces associated with Vander Waals forces and electrostatic charge. The total potential energy can be expressed as:

$$E_{pot} = \Sigma V_{bond} + \Sigma V_{ang} + \Sigma V_{torsion} + \Sigma V_{vdW} + \Sigma V_{ele} + \ldots$$

Its calculation is the main culprit in making MD simulations slow.

Pair wise and Many-Body Potentials:

In pair wise potentials, the total potential energy is calculated from the sum of energy contributions between an atomic pair. An example of such a pair potential is the non-bonded Lennard–Jones potential used for calculating van der Waals forces.

In many-body potentials, the potential energy includes the effects of three or more particles interacting among themselves. In simulations with pairwise potentials, a global interaction exists in the system, but the thing is that they occur only through pairwise terms. In case of many-body potentials, it's difficult to get the potential energy by a sum over pairs of atoms, as these calculations are done explicitly as a combination of higher-order terms. For example, the Tersoff potential and the most widely used embedded-atom method (EAM).

Semi-Empirical Potentials:

It makes use of the matrix representation from quantum mechanics. The matrix is then diagonalized to determine the occupancy of the different atomic orbitals, and empirical formulae are used to determine the energy contributions of the orbitals.

Polarizable Potentials:

It includes the effect of polarizability, means by calculating the partial charges obtained from quantum chemical calculations. This allows for a redistribution of charge between atoms responding to the local chemical environment. For systems like water and protein better simulation results can be obtained by introducing polarizability.

Ab-initio Quantum-Mechanical Methods:

The amount of information Ab-initio calculations produce can't be obtained from empirical methods, such as density of electronic states or other electronic properties.

The unique advantage of using ab-initio methods is the ability to study reactions that involve breaking or formation of covalent bonds, which correspond to multiple electronic states.

Another factor that affects total CPU time required by a simulation is the size of the timestep required for integration which is same as the time length between evaluations of the potential function.

The time step must be chosen small enough to avoid discretization errors. Typical time steps used for classical MD are in the order of 1 femtosecond (10^{-15} s). Proper time integration algorithm should be implemented to achieve optimum simulation time.

3.2.3 Algorithms in Molecular Dynamics [18,27]:

The engine of a molecular dynamics program is its time integration algorithm. Time integration algorithms are based on finite difference principles, which involve discretization of on a finite grid, the time step Δt being the distance between consecutive points. Finding the positions and some of their time derivatives at an instant t, the integration scheme gives the same quantities at a later time $t+\Delta t$. By iterating the procedure, the time evolution of the system can be followed for long times. The schemes are approximate and there are errors associated with them which can be reduced by decreasing Δt.

Two popular integration methods for MD calculations are the Verlet algorithm and predictor-corrector algorithms. Out of these two Verlet algorithm is mostly used. In this case, the position of a particle at any time t is given by:

$$V(t) = \{r(t+\Delta t) - r(t-\Delta t)\}/\{2\Delta t\} \quad \text{(iii)}$$

Where V (t) = Velocity of a particle at time t.

R (t) = position of a particle at time t.

Δt = Small change in time.

The predictor-corrector algorithm comprises of three steps

- Step 1: Predictor: From the positions and their time derivatives at time t, one 'predicts' the same quantities at time $t+\Delta t$ by means of a Taylor expansion. One such quantity is acceleration.
- Step 2: Force evaluation: The force is computed by taking the gradient of the potential at specified locations. The deviation between the resulting acceleration and the predicted acceleration gives error.
- Step 3: Corrector. This error signal is used to 'correct' positions and their relative derivatives.

In all kinds of molecular dynamics simulations, the simulation box size must be sufficient enough to avoid surface defects. Boundary atoms have fewer neighbors than atoms inside resulting surface effects in the simulation to be much more important than they are in the real system. Most of the time Boundary conditions treated by choosing fixed values at the edges, or by the process of employing periodic boundary conditions where the particles interact across the boundary and can move from one end to another end.

3.2.4 Applications of MD simulation [17]:

- For simulation and study of bio-molecular systems like protein synthesis and characterization.
- Designing of drugs in pharmaceutical industry to test properties of a molecule without even synthesizing it.
- Study of the effect of particles like neutrons and ion irradiation on solid surfaces.
- It has wide range of applications in materials sectors too where experiments relating any problem are very difficult to perform in laboratory conditions.
- It is also used to study various kind of properties of metals, non-metals and alloys like fatigue properties, tensile properties, deformation behavior, high temperature behavior etc.

3.3 LAMMPS & VMD[17,18,19]

- LAMMPS is an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator. This is the basic code required to do materials simulation.
- LAMMPS consists of potentials for soft materials and solid-state materials and many more kinds of materials.
- LAMMPS can be used to model atoms or as a parallel particle simulator at the atomic, meso, or continuum scale.
- LAMMPS makes use of MPI(Message Passing Interface) for parallel communication and is free, open-source software, distributed under the terms of the GNU General Public License[18].
- For computational efficiency LAMMPS uses neighbor lists to keep track of particles present at nearby location. The lists are optimized for systems with particles that are repulsive at small distances, resulting the local density of particles never becomes too large[17].

- This code is written with the help of c++. The designing structure of the code is so flexible that it can be easily modified and extended with new applications.
- A combination of pre and post-processing tools are also packaged with LAMMPS, some of which can convert input and output files to/from formats used by other codes.
- VMD is a molecular visualization/graphics program designed for the display and analysis of molecular assemblies.
- VMD can simultaneously and spontaneously display any number of structures using a wide variety of rendering styles and coloring method [19].
- VMD provides a complete graphical user oriented interface for program control, as well as a text interface using the Tcl embeddable parser to allow for complex scripts with variable substitution, control loops and function calls [19].
- It is open source code.

In this project work, all the simulations have been performed using LAMMPS coding and resulting models and structures have been analyzed and processed using VMD Visualization program.

3.4 Simulation Procedures

3.4.1 Procedures:

- In order to perform a simulation task, first we have to download LAMMPS software in our personal computer, which is itself a free source and can be accessed from Sandia National Laboratories website.
- Three basic files or components are required for running any simulation. They are as follows:
    a) In file (program file to create models and performing simulation)
    b) Potential file (contains data about inter atomic bond energy and force field between atoms)
    c) Executable file (lmp_win_no-mpi.exe ,required to run the commands in the in file)
- The next step is to open command prompt screen (dos environment) by typing “cmd” in address bar or in start icon.
- Then the screen will display the path address in which all the aforementioned files are present.
- After that next to the path address type lmp_win_no-mpi.exe< in file name then press enter.
- Then automatically the in file will be executed by the .exe file and if there is any error in the in file then it will be displayed in the command prompt screen and subsequent rectification will be required.

3.4.2 Output of Simulation:

- After successful running of the in file, we will get three out-put files as follows:
    a) DUMP file (containing the atomic co-ordinates of the final structure after simulation and also for deformation studies it contains the stress component values)
    b) Log file (containing thermodynamic data e.g. temperature, pressure, volume, and total energy after a particular no of steps)
    c) Log. lammps file
- Now to see the final structure of our experimented sample after simulation, we have to open dump file containing atomic co-ordinates, through VMD software which need to be installed in the system separately.
- VMD has three parts.
    a) VMD Main
    b) Display Screen
    c) Program Screen

Necessary required adjustments to the finally achieved structure like change of color, display format (Atomic or point etc.), graphics representation styles can be done through VMD main. In display screen we see the image of the final structure. In the program screen, any changes that we do in VMD main and final results are displayed accordingly.

Chapter-4

Results & Discussions

During the execution of this simulation work, the various simulations procedures and analysis that has been carried out are as follows:

a) Creation of crystalline model of pure copper and subsequently indenting the crystal at a definite strain rate and temperature.
b) Creation of Cu-Ni thin films of varying thickness of Nickel layer on a fixed thickness of Copper and subsequent indentation of thin film at a particular strain rate and temperature.
c) Indentation of Cu-Ni thin films of a constant thickness varying strain rate and temperature. When simulations are being done at varying thickness of Nickel coatings, loading rate and temperature parameters are kept constant i.e., 5.0 m/s and 300.0 K respectively. Similarly when simulations are done at varying loading rates and varying temperatures the other two parameters are kept constant.
d) VMD snapshots are taken for the indentation process.
e) Load-Displacement curves were also studied for all the simulations performed.

4.1 Creation of Pure Copper crystal and indentation procedure

Here purpose this simulation is to create a pure copper crystal with a fixed dimension of 140Å* 100Å *140 Å and subsequently indenting the created crystal to obtain Load-Displacement curves, so that it can be compared with those obtained after applying Nickel coatings of varying thickness over same thickness of Copper. The indenter used for the process of nano-indentation is of diameter of 60Å which kept at distance of 5Å over the surface to be indented.

The in file which contains all the commands to create a model of pure copper and to indent it subsequently at a given strain rate (i.e. 0.05 Å/ps) and temperature (i.e. 300K) is given below

 # This program is for performing nano indentation of 3d-crystal lattice of copper

```
units           metal
echo                    both
atom_style      atomic
dimension           3
boundary        p s p
region          box block 0 140 0 100 0 140  units box
create_box          1 box
lattice       fcc 3.61
region          cu block 0 140 0 100  0 140 units box
create_atoms    1 region cu units box
timestep        0.002
pair_style      eam/alloy
pair_coeff          * * Cu_zhou.eam.alloy Cu

# Energy Minimization
minimize        1.0e-4 1.0e-5 10000 10000

# rigid boundary
region    1 block 0 140 0 25 0 140 units box
group     anvil1 region 1
```

```
region      2 block 0 25 0 100 0 140 units box
group       anvil2 region 2
region      3 block 115 140 0 100 0 140 units box
group       anvil3 region 3
group       anvil union anvil1 anvil2 anvil3
group       mobile subtract all anvil
dump 1 all atom 1000 dump.indent8_3d_unload.dump.lammpstrj
log log5050_indent8_3d_voidless_unload.dat
# initial velocities
compute             new mobile temp
velocity            mobile create 300 482748 temp new
fix                 1 mobile  nvt temp 300.0  300.0 0.05
fix                 2 anvil setforce 0.0 0.0 0.0
# assigning velocity to the indenter in y direction/loading direction
variable        y equal "135-step*dt*0.05"
print           "y is $y"

# indenter position and radius at onset of loading
fix             4 mobile indent 1000.0 sphere 70 v_y 70 30.0 units box
thermo      100
thermo_style   custom step temp  v_y f_4[1] f_4[2] f_4[3]
run                 150000
```

This in file can be saved with any name as it is user defined in the same folder containing the potential file and .exe file to run a simulation.

Three regions each of 25Å are defined (i.e. region1, region2, region3) which are subsequently grouped as anvil1, anvil2, anvil3 respectively which are again grouped into anvil by using union command. This anvil region remains rigid while simulation proceeds therefore it is being subtracted from the entire model and the remaining region is named as mobile where all the deformation during the process of indentation takes place. A typical model for the simulation of nano-indentation is shown below.

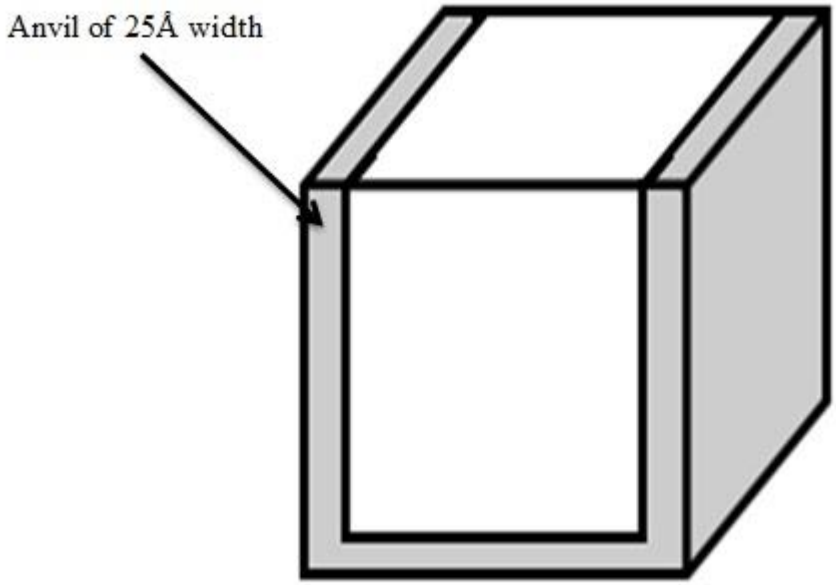


Fig.4.1 Schematic representation of a simulation box.

Time step used for each iteration is 0.002 ps. Indentation is performed until the required indentation depth is achieved. Here in case of pure copper indentation depth is kept as 10 Å.

Number of iteration required to complete a simulation depends upon indentation depth required and strain rate at which indentation has to be performed. For the case of pure copper indentation depth is 10 Å. Total distance to be travelled by indenter tip is the sum of distance of separation from material surface and indentation depth. Here in this case that distance is 5 Å +10 Å =15 Å. Time required in covering this distance for the indenter tip with the specified loading rate (i.e. 0.05 Å /ps) is = 15/0.05= 300 pico seconds.

Therefore total number of iteration = time required / time step = 300/0.002= 150000

After successful completion of simulation, we get the final indented structure of pure copper crystal which can be viewed from different angle by rotating the axis. VMD snapshots for the pure copper crystal after completion of simulation are illustrated below in Fig 4.2. This figure shows indentation shape of the 30Å radius spherical indenter by green line and edge dislocation by a blue line. Sequential VMD snapshots of the same copper block after every 50 ps is shown in the Fig. 4.3.

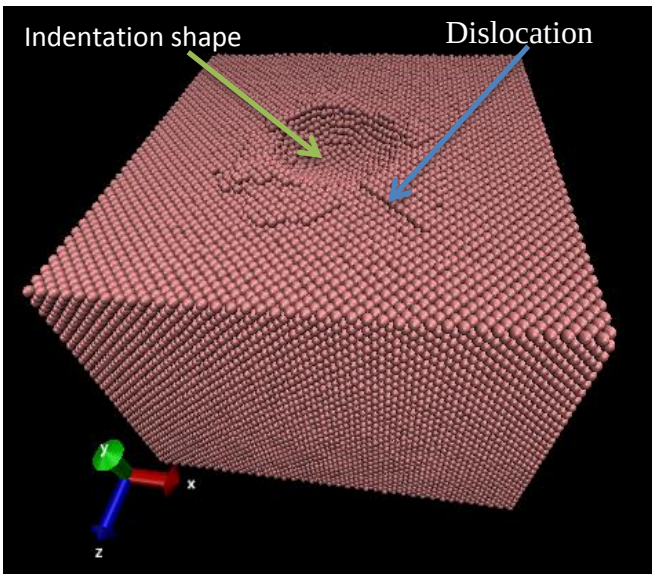


Fig 4.2 VMD Snapshot of the indented pure Cu sample (140Å*100 Å*140 Å) after 300 ps (full simulation) with a loading rate of 0.05 Å/ps and 300K

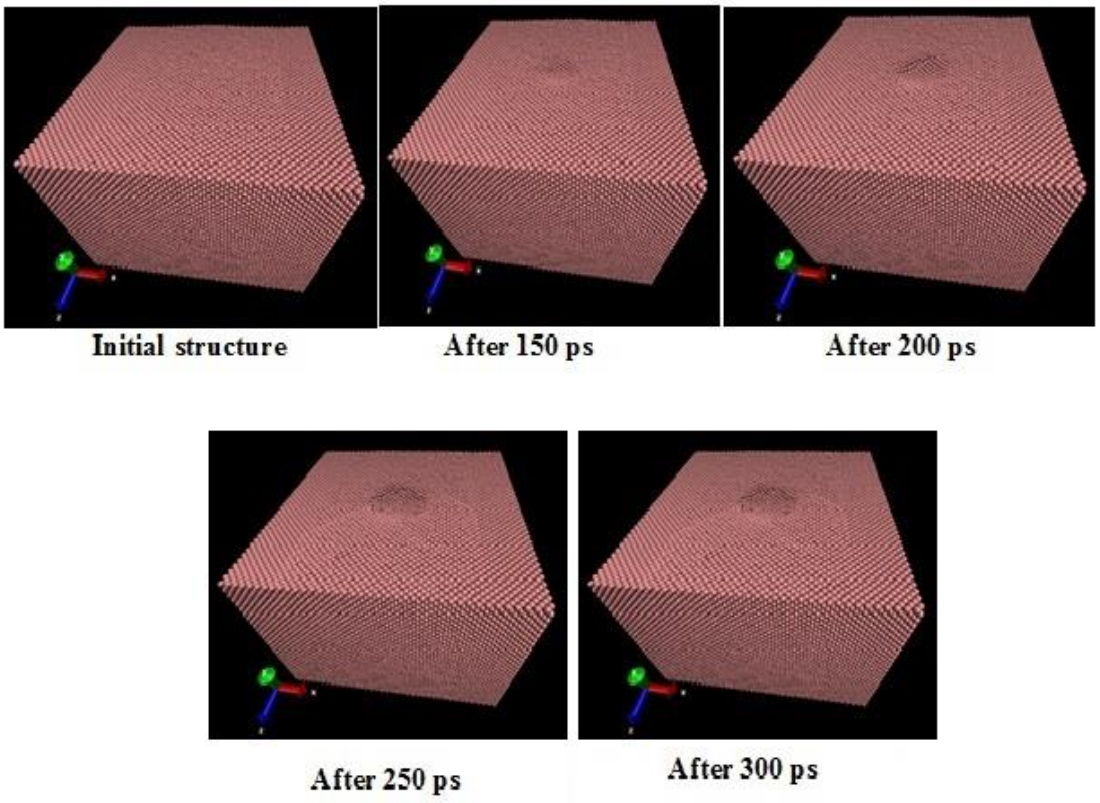


Fig. 4.3 Sequential VMD snapshots of Nano-indentation of pure copper block (140Å*100 Å*140 Å)

The load vs displacement curve is also obtained using Origin 8 software and is plotted in Fig. 4.4 showing increasing load. Sudden drops in load value can be attributed to the nucleation of dislocation. Load value is calculated by multiplying the stress value obtained in the log file by 1.6 so that it gets converted from eV (electron volt) to nN (nano Newton).

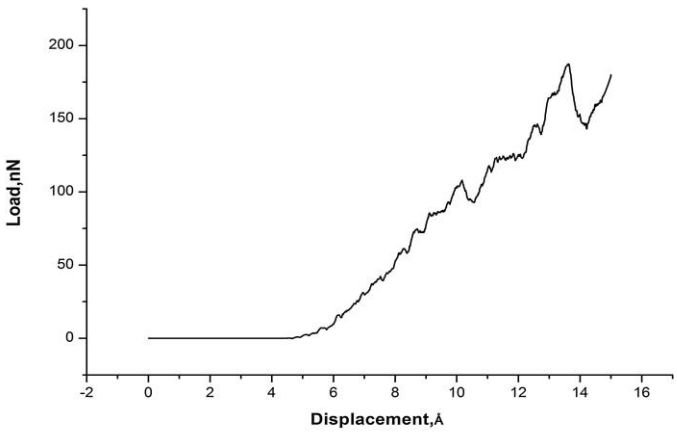


Fig. 4.4 Load-Displacement Curve for nano-indentation of pure copper (140Å*100 Å*140 Å) and a loading rate of 0.05Å/ps and 300K

4.2 Creations of Cu-Ni thin films & Indentation Procedures

While creating Cu-Ni thin films one thing has to be kept in mind that is the dimension of underlying Copper should remain unchanged. Only the thickness of Ni layer over Cu is to be varied as per our requirement. The various Ni layer thickness used in this work are 6Å, 20 Å, 50 Å. While varying the Nickel layer thickness other two parameters for the simulations (strain rate & temperature) are kept fixed.

The in file code for creating a Cu-Ni thin film with 6Å thick Ni layer and subsequently indenting the same is as below.

 # in file for creation of Cu-Ni thin film with Ni layer of 6Å & indentation of the same with a strain rate of 0.05Å/ps and temperature of 300K

```
units           metal
echo            both
atom_style      atomic
dimension       3
boundary        p s p
region          box block 0 140 0 106 0 140  units box
create_box      2 box

lattice         fcc 3.61
region          Cu block 0 140 0 100  0 140 units box
create_atoms    1 region Cu units box
group           substrate region Cu
```

Creates a 3-Dimensional block with 2 boxes within it

Creates Copper block and groups it as substrate

```
lattice        fcc 3.52
region         Ni block 0 140 100 106 0 140 units box
create_atoms   2 region Ni units box
group          deposit region Ni
group          entire union substrate deposit
timestep       0.002
pair_style     eam/alloy
pair_coeff     * * CuNi.set Cu Ni
```

Creates Nickel block and groups it as deposit and further groups the substrate and deposit as entire

```
# Energy Minimization
minimize   1.0e-3 1.0e-6 1000 1000
```

```
# Rigid boundary
region   1 block 0 140 0 25 0 140 units box
group    anvil1 region 1
region   2 block 0 25 0 106 0 140 units box
group    anvil2 region 2
region   3 block 115 140 0 106 0 140 units box
group    anvil3 region 3
group    anvil union anvil1 anvil2 anvil3
group    mobile subtract entire anvil
```

Defines the anvil regions and group them into single name as anvil and subtracts it from entire, naming the rest as mobile

```
dump             1 entire atom 1000 dump.CuNi_thin_film.lammpstrj
dump_modify      1 scale no
log logCu_Ni_thinfilm.data
```

```
# Initializing Velocity
compute    new mobile temp
velocity          mobile create 300 8728007 temp new
fix               1 mobile  nvt temp 300.0  300.0  0.05
fix               2 anvil setforce 0.0 0.0 0.0

# assigning velocity to the indenter in y direction---loading
variable   y equal "141-step*dt*0.05"
print      "y is $y"

# Indenter position and radius at onset of loading
fix               3 mobile indent 1000.0 sphere 70 v_y 70 30.0 units box
thermo       100
thermo_style   custom step temp c_new  v_y f_3[1] f_3[2] f_3[3]
run         80000
```

This is the basic program code in LAMMPS. Any modifications can be done in this code as per the requirements of our simulation. For example if we want to change the Nickel layer thickness from 6Å to 20 Å and 50 Å then this can be done in the upper part of the code where the box dimensions are given for creation of Cu substrate and Ni deposits and everything else will remain unchanged. But when we change the thickness of the Ni layer then depth of indentation gets changed as it have to be exactly half i.e. 50% of the thickness of the Ni deposit. Therefore when we change the Ni layer thickness from 6 Å to 20 Å, the indentation depth changes from 3Å to 10Å thus increasing the total distance to be travelled by the indenter tip from 8Å to 15Å which increases the time requirement and hence the

number of iterations required to complete the simulation. Therefore number of iterations has to be calculated carefully in every process.

When it is required to change the loading rate of indentation, it can be done in the lower part of the code in the variable command while assigning velocities. As in previous case here also repeated calculations has to be performed to calculate number of indentation as the velocity is being changed. As indenter velocity increases the number of iterations required to complete a simulation will definitely reduce. Here in this project work we have performed simulation using three different loading rates keeping the Ni layer thickness and temperature unchanged (20Å and 300K respectively). Three different loading rates used in this project works are 0.05 Å/ps, 0.2 Å/ps, and 0.5 Å/ps.

The required changes in case of temperature change can be performed in the lower part of the code fix command of the mobile region. Since temperature change does not involve any changes in loading rate or Ni layer thickness the number of iterations required to complete a simulation will remain as it is in the previous case. The Ni layer thickness is kept constant at 20 Å and loading rate is kept as 0.5 Å/ps. Three temperature values used in this project work are 300K, 100K, and 50K.

4.3 Comparison of Pure Copper and Cu-Ni thin film

4.3.1 VMD Snapshots:

The VMD snapshots of the initial structures before indentation of both pure copper and Ni coated copper are shown below in Fig. 4.5.

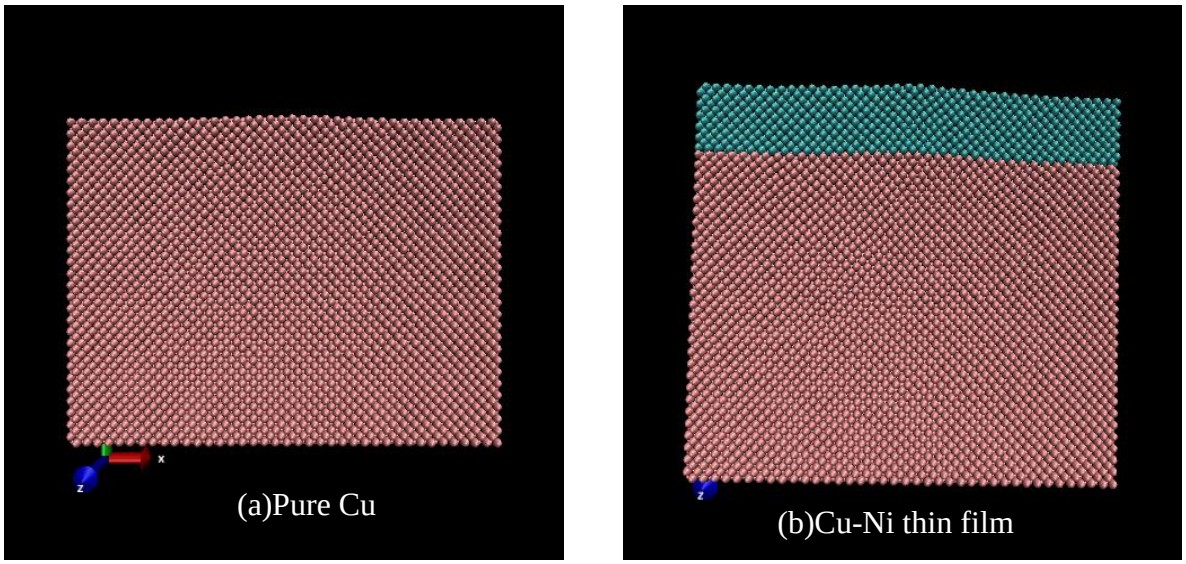
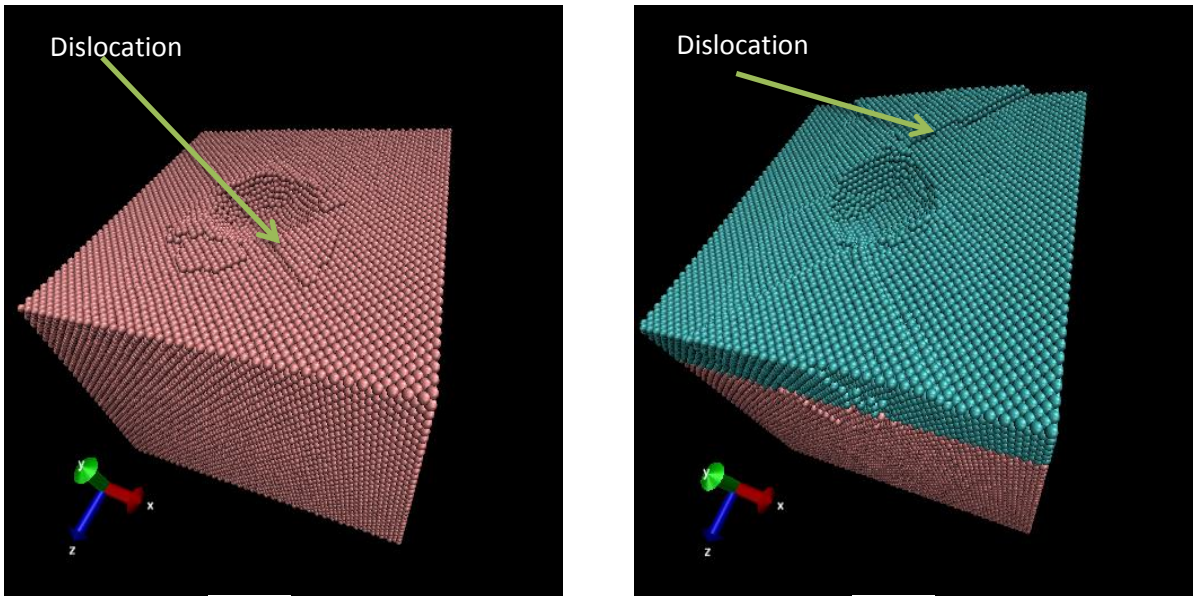


Fig. 4.5 VMD Snapshots of initial structure of (a) Pure Cu and (b) Cu-Ni thin film



(a) **(b)**

Fig. 4.6 VMD Snapshots of indented surface of (a) Pure Cu and (b) Cu-Ni thin film at loading rate of 0.05Å/ps and 300K

The illustrated figures in the previous page show two kinds of structures. Fig. 4.5 shows relaxed configuration of pure copper and Cu-Ni bilayer before the start of indentation. The underlying pink atoms are copper atoms and the deposited blue atoms are Nickel atoms. Fig. 4.6 shows VMD snapshots of deformed surface after nano-indentation. In both the cases of pure copper and Cu-Ni bilayer, formation of dislocation and slip lines can be observed.

4.3.2 Load-Displacement Curves:

The Load-Displacement data in terms of absolute displacement in Å is displayed in a Table 4.1 and the corresponding Load-Displacement curve is plotted for nano-indentation of pure copper in Fig. 4.7.

Sl. No	Displacement(Å)	Load(nN)
01	5	0
02	6	21.0221
03	7	20.5074
04	8	51.1070
05	9	90.0171
06	10	100.5628
07	11	107.6442
08	12	153.3864
09	13	165.2347
10	14	155.8456
11	15	185.26624

Table 4.1 Load-Displacement data for pure copper at a loading rate of 0.05Å/ps and 300K

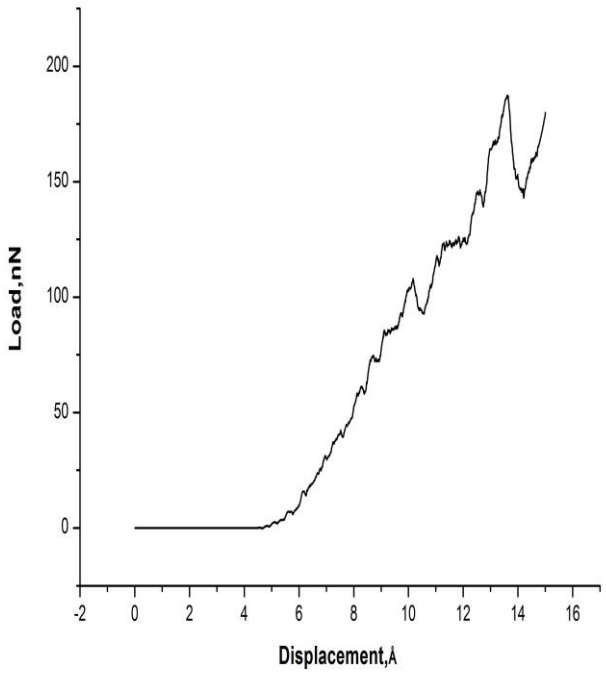


Fig. 4.7 Load-Displacement curve for pure copper at a loading rate of 0.05Å/ps and 300K

Similar data table and curves are shown below for a Cu-Ni thin film with thickness of Ni layer 20Å and at a loading rate of 0.05Å.ps. This particular thickness is selected as comparison of Load-Displacement curve of pure copper can be done with this as the indentation depth is same in both the case i.e. 10Å.

Sl.No	Indenter Displacement, Å	Load,nN
1	5	40.0755
2	6	112.0461
3	7	142.9304
4	8	140.9635
5	9	124.1322
6	10	154.0982
7	11	183.5635
8	12	200.0309
9	13	251.9027
10	14	225.8176
11	15	229.3216

Table 4.2 Load-Displacement data for Cu-20Ni at a loading rate of 0.05Å/ps and 300K

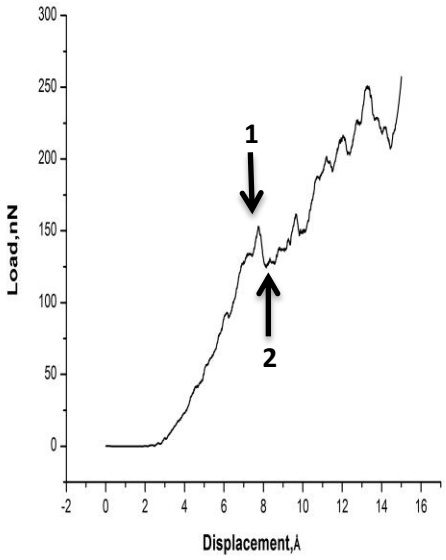


Fig. 4.8 Load-Displacement curve for Cu-20Ni at a loading rate of 0.05Å/ps and 300K

In both the Tables (Table 4.1 and Table 4.2) of Load-Displacement data, it can be clearly seen that the load values increases which are reflected in corresponding plots i.e. Fig 4.7 and Fig.4.8.

In the data obtained for both the cases of pure copper and Cu-Ni thin film we can clearly see that the load gradually increases as the displacement of indenter tip increases or in other way as it enters more into the materials. In both the plots this can be seen. To certain extent deformation behaviour is elastic. Consider the plot in Fig. 4.8, in that plot up to point 1 the deformation can be considered elastic which can be recovered during unloading of indenter. This is the first stage of indentation process and at that point the first inelastic response is recorded. First considerable plastic deformation and which is permanent occurs at a indenter displacement of about 8Å which causes the load drop between point 1 and 2. This is attributed to the nucleation of dislocations in the Nickel layer near the surface along {111} slip planes [26].

Comparison of Load-Displacement curves for pure copper and Cu-Ni bilayer is shown in the following figure.(Fig. 4.9)

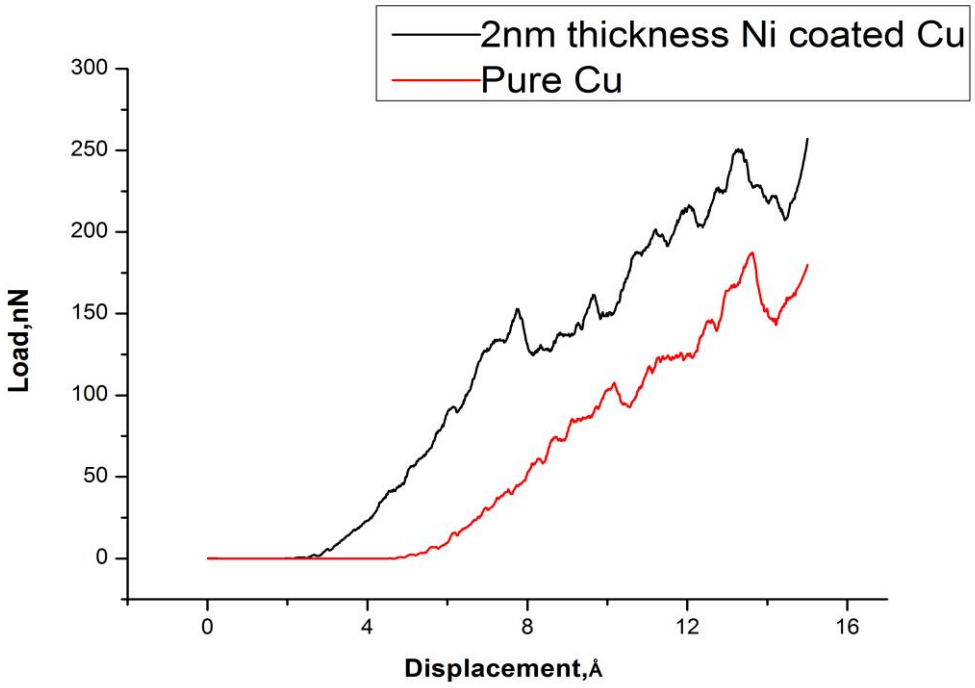


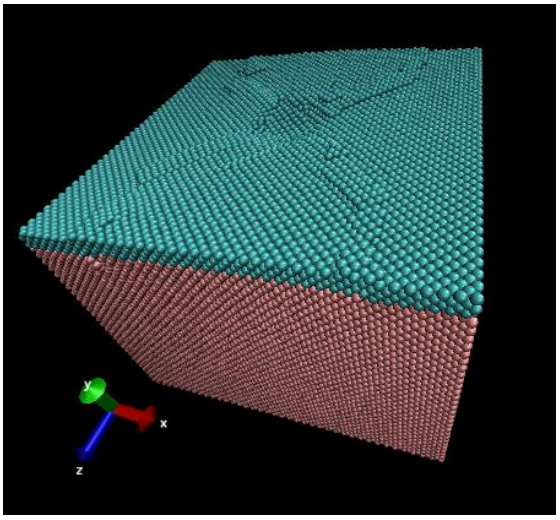
Fig. 4.9 A comparison of the Load-displacement curves of pure copper and Cu-Ni bilayer at a loading rate of 0.05Å/ps and 300K

It is apparent from the Load-Displacement curve comparison in Fig.4.9, that Cu-Ni thin films are significantly strengthened by applying Ni coatings over the underlying copper substrate. Because first of all Ni hardness is significantly higher than that of underlying Copper. Both Cu and Ni have FCC structures with lattice parameter as 3.61Å and 3.52Å respectively. They form a coherent interface with certain amount of coherency strain. This coherency strain arises due to the misfit between FCC Copper and Nickel lattice which is approximately 2.7 % [26]. Coherency strains have to be applied in order to accommodate this misfit and obtain a coherent interface. Dislocations are generated on the top Nickel layer and propagate through (111) FCC interface into Cu. Although dislocations propagate through interface, it acts as a strong barrier. This effect contributes to strain hardening of nano-layered materials in a considerable amount.

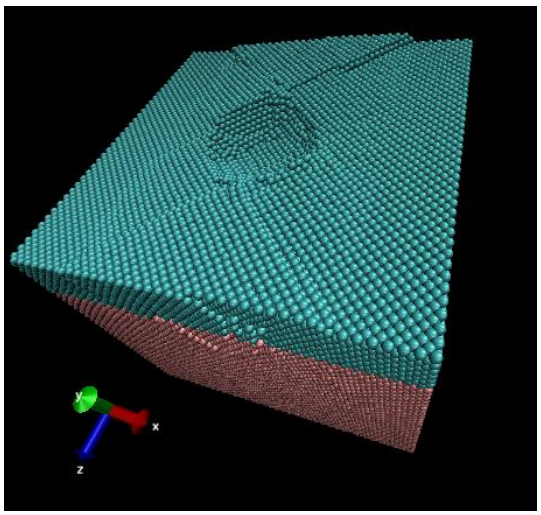
4.4 Effect of thickness of deposited Ni layer

As mentioned earlier simulations have been performed at varying thickness of deposited Ni layer. Various thicknesses used are 6Å, 20 Å, 50 Å.

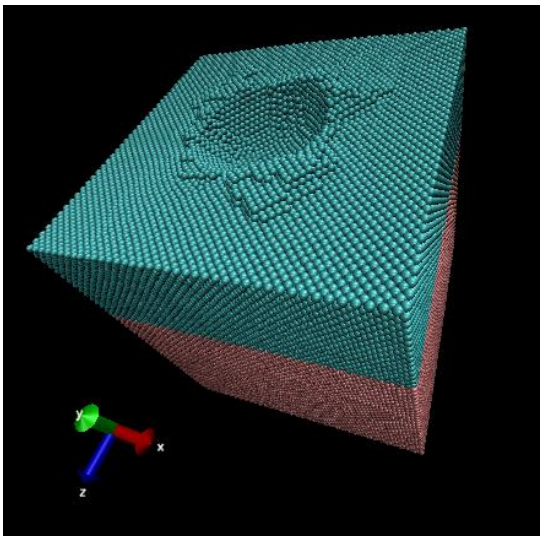
VMD snapshots of the finally indented surface of each of these thicknesses are illustrated below.



(a)Cu-6Å Ni



(b)Cu-20Å Ni



(c)Cu-50Å Ni

Fig. 4.10 VMD snapshots of Cu-Ni bilayer at different thickness of Nickel coating (a) 6Å, (b)20 Å, (c)50 Å at loading rates of 0.05 Å/ps and temperature of 300K.

The Load-Displacement data for Cu-Ni thin film with 20Å Ni thickness is already shown in Table 4.2. The Load-Displacement data for Cu-Ni thin film with 6Å and 50Å Ni thickness are shown in Table 4.3 and Table 4.4 respectively.

Sl.No	**Indenter Displacement, Å**	**Load,nN**
1	5	32.4009
2	6	70.4373
3	7	99.5892
4	8	126.1351

Table 4.3 Load-Displacement data for indentation of 6Å Ni over Cu substrate at a loading rate of 0.05Å/ps and 300K

Sl.No	Indenter Displacement, Å	Load,nN
1	5	6.0242
2	6	56.5375
3	7	81.9636
4	8	98.3988
5	9	179.2792
6	10	162.2803
7	11	187.7180
8	12	219.9317
9	13	285.9795
10	14	300.1780
11	15	263.1040
12	16	316.9013
13	17	273.9042
14	18	316.3553
15	19	385.5836
16	20	395.9963

Table 4.4 Load-Displacement data for indentation of 50Å Ni over Cu substrate at a loading rate of 0.05Å/ps and 300K

The comparison of the Load-Indentation curves for various thicknesses of Ni layer over Cu substrate is illustrated in the Fig.4.11. In all of the cases the Load value is increasing with indenter displacement and all the curves of Ni coated Cu are lying over the curve of pure Cu. The increase in Load at small indentation depth is more pronounced for 20Å (2nm) Ni coated Cu as compared to other two thicknesses values.

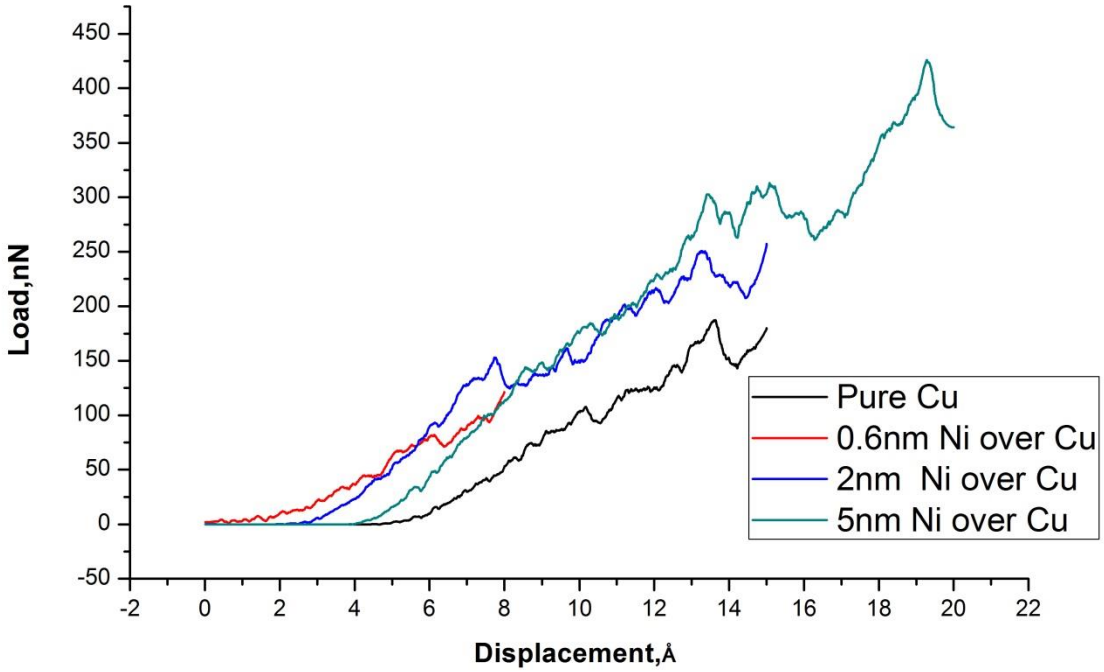
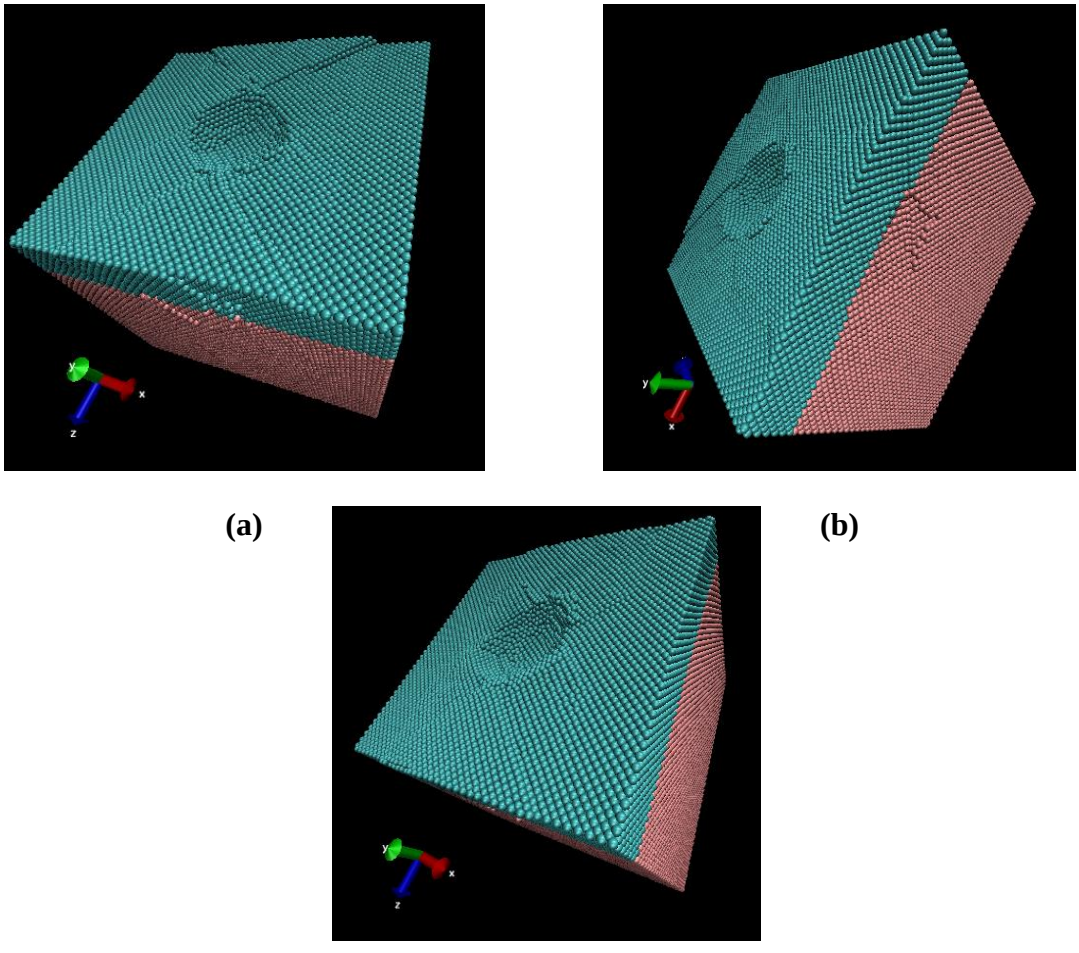


Fig.4.11 Comparison of Load-Displacement curves of varying thickness (0.6nm, 2nm, 5nm) of Ni layer on Cu substrate at loading rate of 0.05Å/ps and 300K

4.5 Effect of loading rates

The various loading rates used for the process of nano-indentation are 0.05Å/ps, 0.2Å/ps and 0.5Å/ps (5m/s, 20m/s, 50m/s). The dimension of the copper box is kept fixed as 140 Å*100 Å*140 Å as mentioned earlier. Along with that the thickness of coated Ni layer is also kept fixed as 20 Å and temperature as 300K for all the three loading rates.

Fig.4.12 shows the VMD snapshots of Cu-Ni bilayer thin film of the mentioned dimension at three varying loading rates. All the VMD snapshots shows indentation shape at the center of the surface and edge dislocations originated due to deformation.



(a) **(b)**

(c)

Fig. 4.12 VMD snapshots of Cu-Ni bilayer thin film with loading rates of (a) 0.05Å/ps (b) 0.2 Å/ps (c) 0.5 Å/ps with Ni layer of 20 Å and temperature of 300K

However any significant statement about effect of loading rates can't be drawn from the Fig. 4.12 as no significant difference is observed in the VMD snapshots. The Load-Displacement data for the loading rate of 0.05 Å/ps is already presented at Table 4.2. The corresponding data tables for loading rates of 0.2 Å/ps and 0.5 Å/ps are presented in Table 4.5 and Table 4.6.

Sl.No	Indenter Displacement, Å	Load, nN
1	5	32.8917
2	6	76.2619
3	7	155.7319
4	8	121.6760
5	9	123.4583
6	10	151.5140
7	11	162.6102
8	12	178.9814
9	13	232.2780
10	14	278.5920
11	15	289.4417

Table 4.5 Load-Displacement data for indentation of 20Å Ni over Cu substrate at a loading rate of 0.2Å/ps and 300K

Sl.No	Indenter Displacement, Å	Load, nN
1	5	29.9810
2	6	88.8212
3	7	82.2480
4	8	112.6372
5	9	146.6919
6	10	178.7346
7	11	193.3939
8	12	187.7218
9	13	240.3192
10	14	326.0002
11	15	285.0006

Table 4.6 Load-Displacement data for indentation of 20Å Ni over Cu substrate at a loading rate of 0.5Å/ps and 300K

From the data represented in the Table 4.5 and Table 4.6, it is clear that load values increases with indenter displacement. But the extent of increase is more at higher loading rates then in lower loading rates. This is displayed in Fig 4.13.

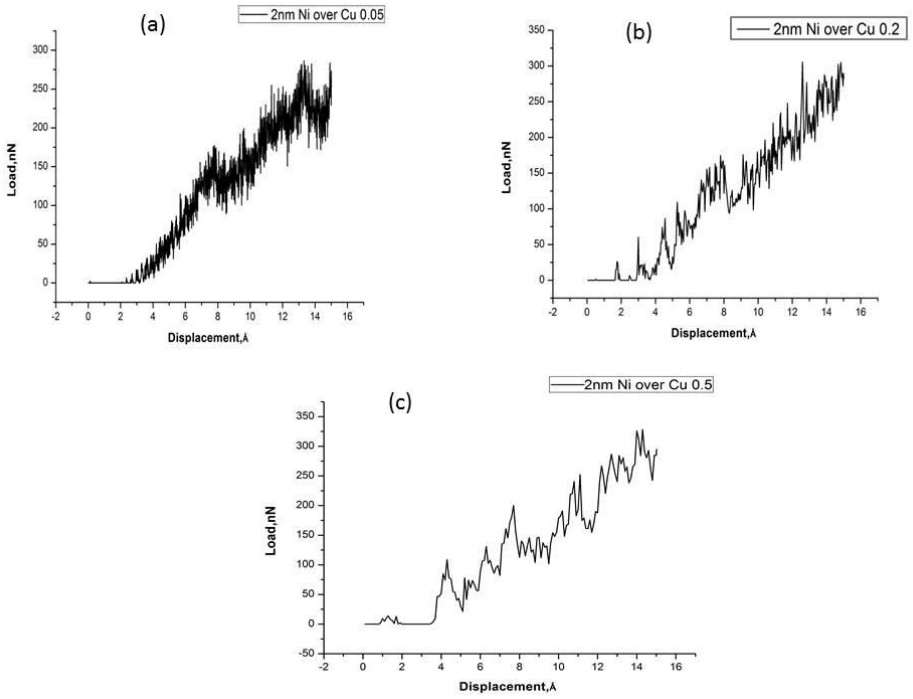


Fig 4.13 Comparison of Load-Displacement curves of varying loading rates (a) 0.05Å/ps, (b) 0.2Å/ps, (c) 0.5Å/ps on Ni layer of thickness 20Å and 300K

Fig.4.13 shows that with increase in loading rates the load requirement also increases. This is because of the larger number of dislocations generated. The enhanced strengthening at higher loading rates can be attributed to higher amount of dislocation-dislocation interaction and interaction of dislocation with the interface.

4.6 Effect of Temperature

As already mentioned earlier simulations are also performed at varying temperature of nano-indentation. Various temperatures used in this project work are 300K, 100K, and 50K.

VMD snapshots of the indented surface of Cu-Ni bilayer are shown in Fig. 4.14.

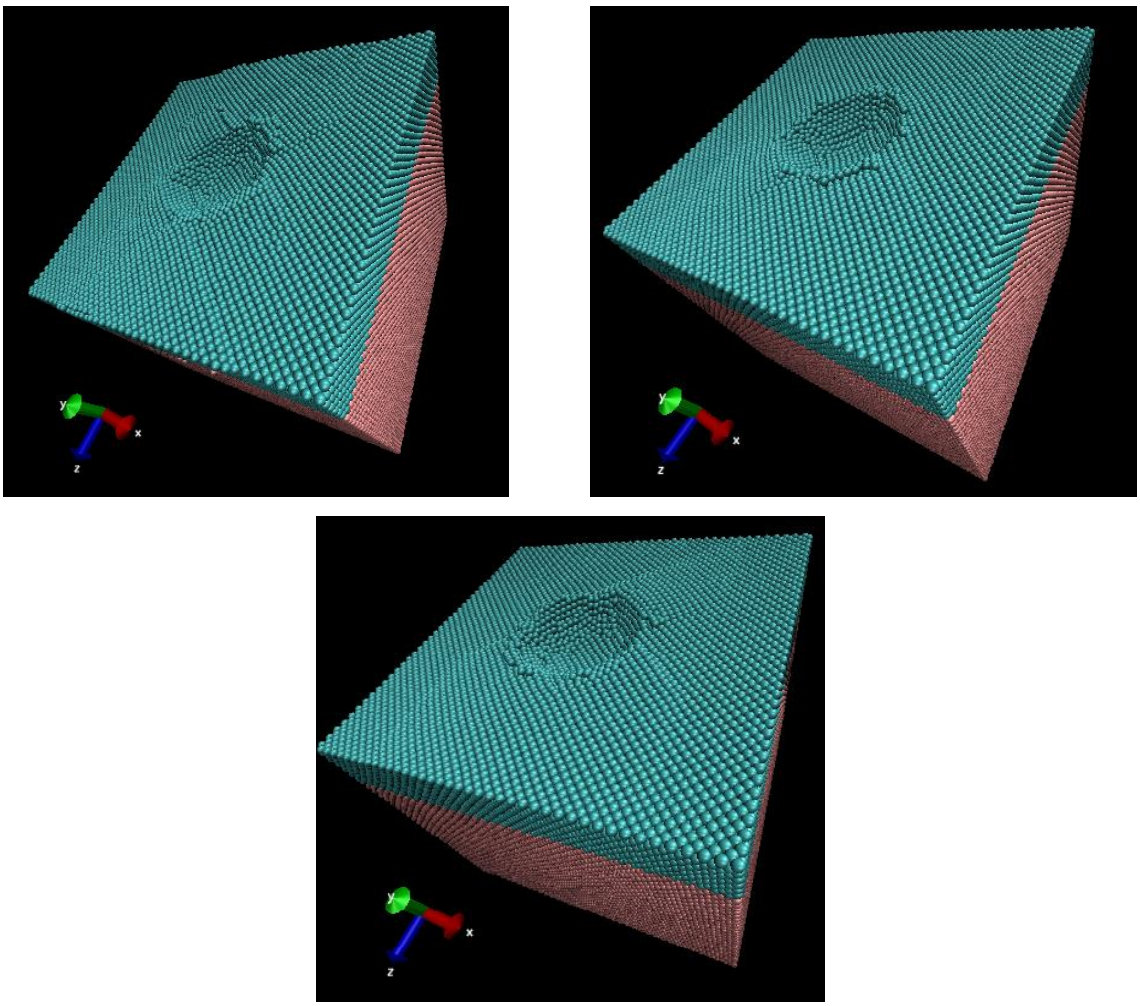


Fig. 4.14 VMD snapshots of Cu-Ni bilayer thin film with temperature of (a) 300K (b) 100K (c) 50K with Ni layer of 20 Å and loading rate of 0.5 Å/ps

Here also any significant statement about effect of temperature can't be drawn from the Fig. 4.14 as no significant difference is observed in the VMD snapshots. The Load-Displacement data for the temperature of 300K is already presented at Table 4.6. The corresponding data tables for temperature of 100K and 50K are presented in Table 4.7 and Table 4.8 respectively.

Sl.No	Indenter Displacement,Å	Load,nN
1	5	37.1680
2	6	79.2270
3	7	101.0739
4	8	141.5582
5	9	193.4273
6	10	148.2525
7	11	161.5359
8	12	231.4391
9	13	235.2600
10	14	311.9646
11	15	326.7314

Table 4.7 Load-Displacement data for indentation of 20Å Ni over Cu substrate at a loading rate of 0.5Å/ps and 100K

Sl.No	Indenter Displacement,Å	Load,nN
1	5	49.0041
2	6	91.4172
3	7	103.1663
4	8	134.3430
5	9	174.7815
6	10	162.9177
7	11	197.1294
8	12	245.6079
9	13	250.4889
10	14	285.5794
11	15	300.0125

Table 4.8 Load-Displacement data for indentation of 20Å Ni over Cu substrate at a loading rate of 0.5Å/ps and 50K

From the data represented in the Table 4.7 and Table 4.8, it is clear that load values increases with indenter displacement. But the extent of increase is more pronounced at lower temperature. This is displayed in Fig 4.15.

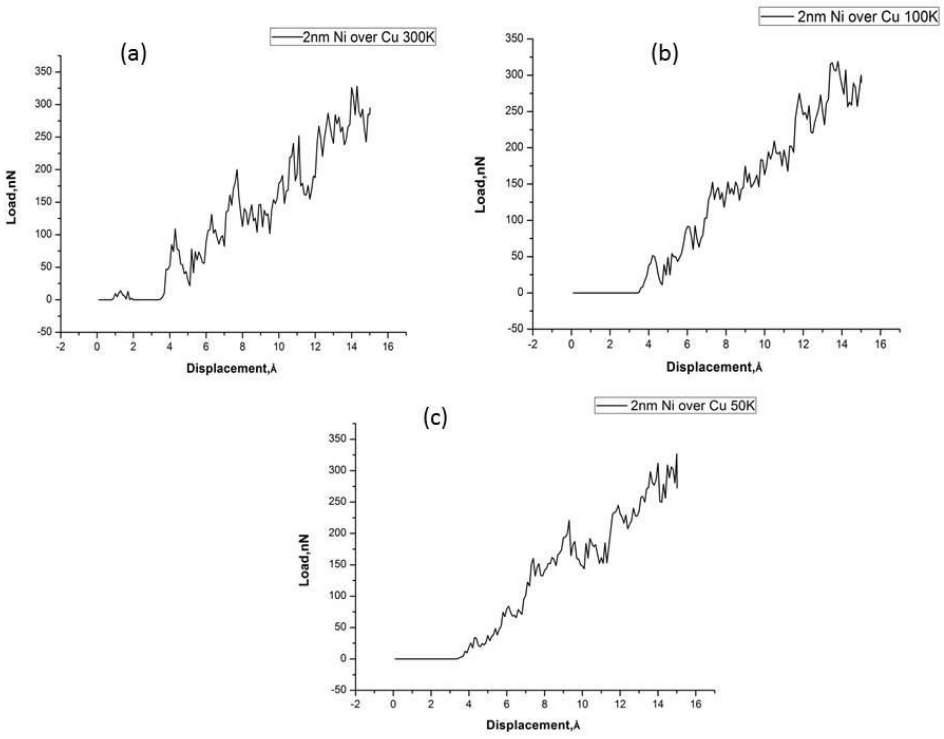


Fig 4.15 Comparison of Load-Displacement curves of varying temperature (a) 300K, (b)100K, (c)50K on Ni layer of thickness 20Å and loading rate of 0.5 Å/ps.

Fig.4.15 shows that with decrease in temperature the load requirement increases. Thus it can be stated as strengthening is more pronounced at lower temperatures. This is because of the material become brittle at low temperature thus enhancing the strengthening mechanism.

5. Conclusions

From the Molecular Dynamics Simulation study of nano-indentation of Cu-Ni thin films and study of the effect of Ni layer thickness, loading rate and temperature on Load-Displacement behaviour we conclude the following;

1. Cu films can be significantly strengthened applying coating of Nickel over the underlying substrate of copper and the effect gets enhanced with increase in thickness specifically at 2nm(20Å).
2. As loading rate during nano-indentation is increased the strengthening effect also enhances significantly.
3. This strengthening of Cu-Ni thin films due to Ni coating is more pronounced at low temperature.

FUTURE WORK:

a) Effect of indenter size i.e. radius of indenter on the behaviour of thin films.
b) Effect of loading angle during indention on the deformation behaviour of thin films.
c) Study of Centro-symmetry parameter and observation of dislocation loops after nano-indention.

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